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A Numerical Method for Heat Equations Involving Interfaces

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Abstract. In 1993, Li and Mayo gave a finite-difference method with second order accuracy for solving the heat equations involving interfaces with constant coefficients and discontinuous sources [Proc. Symp. Appl. Math. Vol. 48, W.Gautschi ed., AMS, 1993, p 311-315]. In this paper, we improve the above result by presenting a finite-difference method which allows each coefficient to be taken different values in different subregions divided by the interface, that is useful in applications. Our method also has second order accuracy.

1. Introduction

Consider the heat equation

$$u_t = (\beta u_x)_x + (\beta u_y)_y, \quad (1.1)$$

where $t \in [a, \infty)$ and $(x, y) \in \Omega$, a rectangular region in R^2 with an irregular interface Γ which divides Ω to two subregions Ω_1 and Ω_2 . The solution $u(x, y, t)$ and its normal derivative $u_n(x, y, t)$ crossing the curve Γ are known to be discontinuous:

$$[u] \equiv u^+ - u^- = \omega(x(s), y(s), t), \quad (1.2)$$

$$[u_n] \equiv u_n^+ - u_n^- = g(x(s), y(s), t), \quad (1.3)$$

where s is a parameter of Γ , the superscripts $+$ and $-$ denote the limiting values of a function from one side in Ω^+ and another side in Ω^- respectively.

In 1993, Li and Mayo[3] gave a finite-difference method with second accuracy for solving (1.1), assuming that f is discontinuous but β is constant. In this paper, we present a finite-difference method for solving (1.1), which allows β to be taken different values in different subregions divided by the interface, and which is useful in applications. More precisely, we assume:

$$\beta(x, y) = \begin{cases} \beta^+, & \text{if } (x, y) \in \Omega^+, \\ \beta^-, & \text{if } (x, y) \in \Omega^-, \end{cases} \quad (1, 4)$$

where β^+, β^- are constants which can be distinct.

We organize the paper as follows: In Section 2, we establish local coordinate systems around the interface. In Section 3, we give the correction terms for the finite-difference method. In Section 4, we show that our method is second accurate. Finally, in Section 5, we give some numerical examples, in which the actual solutions are known, to confirm the theoretical result.

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2. Local Coordinate Systems

We first give local coordinate systems along the interface Γ as [2,3]. When a point on the interface is fixed for the origin, we use the normal direction as the ξ -direction, which has an angle θ with the x -axis. Rotating the ξ -direction by ninety degrees anti-clockwise, we obtain the η -direction. Now we express the curve Γ as a function of the independent variable η locally:

$$\xi = \chi(\eta). \quad (2.1)$$

We express (1.2),(1.3) locally by using the η coordinate:

$$[u] \equiv u^+ - u^- = \omega(\eta, t), \quad (2.2)$$

$$[u_n] \equiv u_n^+ - u_n^- = g(\eta, t), \quad (2.3)$$

where ω, g are known in advance. From

$$g = [u_n] = -\frac{[u_\eta]\chi_\eta + [u_\xi]}{\sqrt{1 + \chi_\eta^2}}. \quad (2.4)$$

Using differentiation w.r.t. η , noting $\chi(0) = 0$, we have:

$$[u_\eta] = \omega_\eta, \quad [u_\xi] = g, \quad (2.5, 2.6)$$

$$[u_{\eta\eta}] = -g\chi_{\eta\eta} + \omega_{\eta\eta}, \quad [u_{\xi\eta}] = \omega_\eta\chi_{\eta\eta} + g_\eta. \quad (2.7, 2.8)$$

Changing (1.1) locally, we have:

$$u_t = \beta u_{\xi\xi} + \beta u_{\eta\eta} + f(\xi, \eta, t), \quad (2.9)$$

which implies

$$[u_{\xi\xi}] = [u_{\xi\xi}]_1 + \left[\frac{u_t}{\beta} \right], \quad (2.10)$$

where

$$[u_{\xi\xi}]_1 = g\chi_{\eta\eta} - \omega_{\eta\eta} - \left[\frac{f}{\beta} \right]. \quad (2.11)$$

In (2.5)-(2.11), all functions in the right-hand sides are known except $\left[\frac{u_t}{\beta} \right]$ in (2.10) which will be explored in the next section.

3. Correction Terms

We first discretize in both of the x -direction and the y -direction by mesh size h :

$$u_{xx} \approx \delta_x u_{i,j} \equiv \frac{1}{h^2} (u_{i-1,j} - 2u_{i,j} + u_{i+1,j}), \quad (3.1)$$

$$u_{yy} \approx \delta_y u_{i,j} \equiv \frac{1}{h^2} (u_{i,j-1} - 2u_{i,j} + u_{i,j+1}). \quad (3.2)$$

We group all the grid points in Ω into two sets. The set S_{reg} consists the regular points, each point in one subregion has no neighbor point in the another subregion. The set S_{irr} consists the irregular points, each point in one subregion has at least one neighbor point in the other subregion. For a regular grid point, the local truncation error of (3.1),(3.2) from $\beta u_{xx} + \beta u_{yy} + f$ is $O(h^2)$. For an irregular grid point, we need add some correction terms in (3.1),(3.2) such that the local truncation error is $O(h)$, therefore the global error of the solution for solving the heat equation is $O(h^2)$ after the discretization of time t in certain way.

At first, we relate the jumps w.r.t. x and y to the jumps w.r.t. ξ and η :

$$[u_x] = [u_\xi] \cos\theta - [u_\eta] \sin\theta, \quad [u_y] = [u_\xi] \sin\theta + [u_\eta] \cos\theta, \quad (3.3, 3.4)$$

$$[u_{xx}] = [u_{xx}]_1 + \left[\frac{u_t}{\beta} \right] \cos^2\theta, \quad (3.5)$$

where

$$[u_{xx}]_1 = [u_{\xi\xi}]_1 \cos^2\theta - 2[u_{\xi\eta}] \cos\theta \sin\theta + [u_{\eta\eta}] \sin^2\theta, \quad (3.6)$$

$$[u_{yy}] = [u_{yy}]_1 + \left[\frac{u_t}{\beta} \right] \sin^2\theta,$$

where

$$[u_{yy}]_1 = [u_{\xi\xi}]_1 \sin^2\theta + 2[u_{\xi\eta}] \cos\theta \sin\theta + [u_{\eta\eta}] \cos^2\theta.$$

By (2.5)-(2.11), all the terms in the right-hand sides of (3.3)-(3.6) are known except $[\frac{u_t}{\beta}]$.

Now we consider an irregular grid point in x -direction, there are four cases:

$$(a) \quad (x_i, y_j) \in \Omega^-, (x_{i+1}, y_j) \in \Omega^+; \quad (b) \quad (x_i, y_j) \in \Omega^+, (x_{i-1}, y_j) \in \Omega^-;$$

$$(c) \quad (x_i, y_j) \in \Omega^+, (x_{i+1}, y_j) \in \Omega^-; \quad (d) \quad (x_i, y_j) \in \Omega^-, (x_{i-1}, y_j) \in \Omega^+.$$

For case(a), let the intersection of the line segment connecting $(x_i, y_j), (x_{i+1}, y_j)$ and Γ is (x^*, y_j) . Using Taylor's series around x^* , we have:

$$\begin{aligned} & \frac{1}{h^2} \{u(x_{i-1}, y_j) - 2u(x_i, y_j) + u(x_{i+1}, y_j)\} \\ &= \frac{1}{h^2} \{[u] + [u_x](x_{i+1} - x^*) + \frac{[u_{xx}]}{2!}(x_{i+1} - x^*)^2\} + u_{xx}^- + O(h), \end{aligned}$$

which implies

$$u_{xx} = \delta_x u_{i,j} + C_x u_{i,j} - \frac{[\frac{u_t}{\beta}](x_{i+1} - x^*)^2}{2h^2} + O(h), \quad (3.7)$$

where

$$C_x u_{i,j} = -\frac{1}{h^2} \{[u] + [u_x](x_{i+1} - x^*) + \frac{[u_{xx}]_1}{2!}(x_{i+1} - x^*)^2\}.$$

Similarly, for case(b), we have

$$u_{xx} = \delta_x u_{i,j} + C_x u_{i,j} + \frac{[\frac{u_t}{\beta}](x_{i-1} - x^*)^2}{2h^2} + O(h), \quad (3.8)$$

where

$$C_x u_{i,j} = \frac{1}{h^2} \{[u] + [u_x](x_{i-1} - x^*) + \frac{[u_{xx}]_1}{2!}(x_{i-1} - x^*)^2\}.$$

For case(c), we have

$$u_{xx} = \delta_x u_{i,j} + C_x u_{i,j} + \frac{[\frac{u_t}{\beta}](x_{i+1} - x^*)^2}{2h^2} + O(h), \quad (3.9)$$

where

$$C_x u_{i,j} = \frac{1}{h^2} \{[u] + [u_x](x_{i+1} - x^*) + \frac{[u_{xx}]_1}{2!}(x_{i+1} - x^*)^2\}.$$

For case(d), we have

$$u_{xx} = \delta_x u_{i,j} + C_x u_{i,j} - \frac{[\frac{u_t}{\beta}](x_{i-1} - x^*)^2}{2h^2} + O(h), \quad (3.10)$$

where

$$C_x u_{i,j} = -\frac{1}{h^2} \{[u] + [u_x](x_{i-1} - x^*) + \frac{[u_{xx}]_1}{2!}(x_{i-1} - x^*)^2\}.$$

Analogously, in y -direction, we also have four cases. We add correction terms such that the local truncation is $O(h)$.

Now using these correction terms in both x - and y - directions, we obtain a system of ordinary differential equations:

$$(u_{i,j})_t = \beta\{\delta_x u_{i,j} + \delta_y u_{i,j}\} + f_{i,j} + \beta \sum_{(x_{i_0}, y^*) \in S_{irr}} \left\{ c_x u_{i,j} + \left[\frac{u_t}{\beta} \right] \frac{\tau_{x_0} (x_{i_0} - x^*)^2 \cos^2 \theta}{2h^2} \right\} \\ + \beta \sum_{(x^*, y_{j_0}) \in S_{irr}} \left\{ c_y u_{i,j} + \left[\frac{u_t}{\beta} \right] \frac{\tau_{y_0} (y_{j_0} - y^*)^2 \sin^2 \theta}{2h^2} \right\} + O(h), \quad (3.11)$$

where $i_0 = i - 1$ or $i + 1$, $j_0 = j - 1$ or $j + 1$. $\tau_{x_0}, \tau_{y_0} = 1$ or -1 according to (3.7)-(3.10). We have

$$\left[\frac{u_t}{\beta} \right] = u_t^- \left[\frac{1}{\beta} \right] + \frac{[u_t]}{\beta^+} = u_t^+ \left[\frac{1}{\beta} \right] + \frac{[u_t]}{\beta^-}, \quad (3.12, 3.13)$$

which imply

$$\left[\frac{u_t}{\beta} \right] = (u_{i,j})_t \left[\frac{1}{\beta} \right] + O(h). \quad (3.14)$$

Using (3.14), we have the following system of ordinary differential equations:

$$(u_{i,j})_t = F(u_{i,j-1}, u_{i-1,j}, u_{i,j}, u_{i+1,j}, u_{i,j+1}) \equiv \\ \frac{\beta(\delta_x u_{i,j} + \delta_y u_{i,j} + \sum_{(x_{i_0}, y^*) \in S_{irr}} c_x u_{i,j} + \sum_{(x^*, y_{j_0}) \in S_{irr}} c_y u_{i,j}) + f_{i,j}}{1 - \sum_{(x_{i_0}, y^*) \in S_{irr}} \beta \left[\frac{1}{\beta} \right] \frac{\tau_{x_{i_0}} (x_{i_0} - x^*)^2 \cos^2 \theta}{2h^2} - \sum_{(x^*, y_{j_0}) \in S_{irr}} \beta \left[\frac{1}{\beta} \right] \frac{\tau_{y_{j_0}} (y_{j_0} - y^*)^2 \sin^2 \theta}{2h^2}}. \quad (3.15)$$

At a regular grid point, the local truncation error of the right-hand side of (3.15) from $\beta u_{xx} + \beta u_{yy} + f$ is $O(h^2)$. In the next section, we will show that at an irregular grid point, the local truncation error is $O(h)$.

Finally, we discretize time t by choosing $\Delta t = h^2$. We use Crank-Nicholson method:

$$u_{i,j,k+1} = u_{i,j,k} + \Delta t (0.5F(u_{i,j-1,k}, u_{i-1,j,k}, u_{i,j,k}, u_{i+1,j,k}, u_{i,j+1,k}) \\ + 0.5F(u_{i,j-1,k+1}, u_{i-1,j,k+1}, u_{i,j,k+1}, u_{i+1,j,k+1}, u_{i,j+1,k+1})), \quad (3.16)$$

which implies the local truncation error for discretizing t is $O((\Delta t)^2)$. (see [1,4].) To solve $u_{i,j,k+1}$ from (3.16), we use S.O.R. iteration with certain parameter ω :

$$u_{i,j,k+1}^{(0)} = u_{i,j,k}, \quad (3.17)$$

and

$$u_{i,j,k+1}^{(n+1)} = (1 - \omega) u_{i,j,k+1}^{(n)} + \omega (u_{i,j,k} + 0.5F(u_{i,j-1,k}, u_{i-1,j,k}, u_{i,j,k}, u_{i+1,j,k}, u_{i,j+1,k}) \\ + 0.5F(u_{i,j-1,k+1}^{(n+1)}, u_{i-1,j,k+1}^{(n+1)}, u_{i,j,k+1}^{(n)}, u_{i+1,j,k+1}^{(n)}, u_{i,j+1,k+1}^{(n)})), n = 1, 2, \dots \quad (3.18)$$

4. Accuracy Analysis

We first show that the denominator of the right-hand side of (3.15) is bounded below and above by positive constants:

Lemma 4.1. Let $D_{i,j} \equiv$

$$1 - \sum_{(x_{i_0}, y_{j_0}) \in S_{irr}} \beta \left[\frac{1}{\beta} \right] \frac{\tau_{x_{i_0}} (x_{i_0} - x^*)^2 \cos^2 \theta}{2h^2} - \sum_{(x^*, y_{j_0}) \in S_{irr}} \beta \left[\frac{1}{\beta} \right] \frac{\tau_{y_{j_0}} (y_{j_0} - y^*)^2 \sin^2 \theta}{2h^2}. \quad (4.1)$$

Then

$$\frac{\min(\beta^+, \beta^-)}{\max(\beta^+, \beta^-)} \leq D_{i,j} \leq 1 + \max(\beta^+, \beta^-) \left| \left[\frac{1}{\beta} \right] \right|, \quad (4.2)$$

where $i_0 = i-1$ or $i+1$, $j_0 = j-1$ or $j+1$. $\tau_{x_{i_0}}, \tau_{y_{j_0}} = 1$ or -1 according to (3.7)-(3.10).

Proof: At first we prove the lower bound. Look at the first summation. In x-direction, we have four cases.

- (a) $(x_i, y_j) \in \Omega^-, (x_{i+1}, y_j) \in \Omega^+$. Then $x_{i_0} = x_{i+1}$, $\tau_{x_{i_0}} = -1$, $\beta = \beta^-$,
and $\beta \left[\frac{1}{\beta} \right] \tau_{x_{i_0}} = 1 - \frac{\beta^-}{\beta^+}$ which is positive iff $\beta^- < \beta^+$.
- (b) $(x_i, y_j) \in \Omega^+, (x_{i-1}, y_j) \in \Omega^-$. Then $x_{i_0} = x_{i-1}$, $\tau_{x_{i_0}} = 1$, $\beta = \beta^+$,
and $\beta \left[\frac{1}{\beta} \right] \tau_{x_{i_0}} = 1 - \frac{\beta^+}{\beta^-}$ which is positive iff $\beta^+ < \beta^-$.
- (c) $(x_i, y_j) \in \Omega^+, (x_{i+1}, y_j) \in \Omega^-$. Then $x_{i_0} = x_{i+1}$, $\tau_{x_{i_0}} = 1$, $\beta = \beta^+$,
and $\beta \left[\frac{1}{\beta} \right] \tau_{x_{i_0}} = 1 - \frac{\beta^+}{\beta^-}$ which is positive iff $\beta^+ < \beta^-$.
- (d) $(x_i, y_j) \in \Omega^-, (x_{i+1}, y_j) \in \Omega^+$. Then $x_{i_0} = x_{i-1}$, $\tau_{x_{i_0}} = -1$, $\beta = \beta^-$,
and $\beta \left[\frac{1}{\beta} \right] \tau_{x_{i_0}} = 1 - \frac{\beta^-}{\beta^+}$ which is positive iff $\beta^- < \beta^+$.

For all cases, a term in the first summation is positive iff $\beta = \min\{\beta^+, \beta^-\}$. Similarly we can show that a term in the second summation is positive iff $\beta = \min\{\beta^+, \beta^-\}$ too. Only the positive terms will reduce the lower bound of the left-hand side of (4.1). So the left-hand side is bounded below by

$$D_{i,j} \geq 1 - 0.5 \left(1 - \frac{\min(\beta^+, \beta^-)}{\max(\beta^+, \beta^-)} \right) - 0.5 \left(1 - \frac{\min(\beta^+, \beta^-)}{\max(\beta^+, \beta^-)} \right) = \frac{\min(\beta^+, \beta^-)}{\max(\beta^+, \beta^-)}.$$

Now we turn to the upper bound which can be proved directly from (4.1):

$$D_{i,j} \leq 1 + 0.5\beta \left| \left[\frac{1}{\beta} \right] \right| + 0.5\beta \left| \left[\frac{1}{\beta} \right] \right| \leq 1 + \max(\beta^+, \beta^-) \left| \left[\frac{1}{\beta} \right] \right|.$$

The lower bound in (4.2) is useful for the stability of the numerical scheme and the upper bound will be used for the following theorem:

Theorem 4.2.

$$F(u_{i,j-1}, u_{i-1,j}, u_{i,j}, u_{i+1,j}, u_{i,j+1}) - (\beta u_{xx} + \beta u_{yy} + f)(x_i, y_j) = O(h), \quad (4.3)$$

where (x_i, y_j) is an irregular grid point in Ω .

Proof: From (3.15), (3.14), (4.2) and (3.11), we have:

$$\begin{aligned} F(u_{i,j-1}, u_{i-1,j}, u_{i,j}, u_{i+1,j}, u_{i,j+1}) &= (u_{i,j})_t = \\ &= \beta(\delta_x u_{i,j} + \delta_y u_{i,j} + \sum_{(x_{i_0}, y^*) \in S_{irr}} c_x u_{i,j} + \sum_{(x^*, y_{j_0}) \in S_{irr}} c_y u_{i,j}) + f_{i,j} \\ &- (u_{i,j})_t \left(\sum_{(x_{i_0}, y^*) \in S_{irr}} \beta \left[\frac{1}{\beta} \right] \frac{\tau_{x_{i_0}} (x_{i_0} - x^*)^2 \cos^2 \theta}{2h^2} + \sum_{(x^*, y_{j_0}) \in S_{irr}} \beta \left[\frac{1}{\beta} \right] \frac{\tau_{y_{j_0}} (y_{j_0} - y^*)^2 \sin^2 \theta}{2h^2} \right) \\ &= \beta \{ \delta_x u_{i,j} + \delta_y u_{i,j} \} + f_{i,j} + \beta \sum_{(x_{i_0}, y^*) \in S_{irr}} \left\{ c_x u_{i,j} + \left[\frac{u_t}{\beta} \right] \frac{\tau_{x_{i_0}} (x_{i_0} - x^*)^2 \cos^2 \theta}{2h^2} \right\} \\ &+ \beta \sum_{(x^*, y_{j_0}) \in S_{irr}} \left\{ c_y u_{i,j} + \left[\frac{u_t}{\beta} \right] \frac{\tau_{y_{j_0}} (y_{j_0} - y^*)^2 \sin^2 \theta}{2h^2} \right\} + O(h) \\ &= (\beta u_{xx} + \beta u_{yy} + f)(x_i, y_j) + O(h), \end{aligned}$$

which proves (4.3).

At a regular grid point, the local truncation error for discretization is $O(h^2)$. At an irregular grid point, the local truncation error is $O(h)$ by Theorem 4.2. The discretization of time is $O((\Delta t)^2) = O(h^4)$. All these imply that the numerical solution has global error $O(h^2)$.

5. Numerical Examples

We choose some examples, in which the actual solutions are known, therefore numerical error computations can be obtained to confirm the theoretical result of our method. We choose

$$\Omega = [-1, 1] \times [-1, 1], \quad t \in [0, \infty], \quad (5.1, 5.2)$$

$$\Omega^+ = \{(x, y) \in \Omega \mid x^2 + y^2 > 1/4\}, \quad \Omega^- = \{(x, y) \in \Omega \mid x^2 + y^2 < 1/4\}, \quad (5.3, 5.4)$$

$$\Gamma = \{(x, y) \in \Omega \mid x^2 + y^2 = 1/4\}. \quad (5.5)$$

The actual solution is known in the case $f = 0$:

$$u(x, y, t) = \frac{1}{t} e^{-\frac{x^2+y^2}{4\beta t}}. \quad (5.6)$$

We give the initial condition when $t = 1$ and boundary condition when x or $y = 1$ or -1 by using formula (5.6). We choose $\omega = 1.75$ in (3.18). For different pairs of β^+ and β^- , in t from 1.0 to 1.5, we obtain the following tables, in each the error is computed by using Euclidean norm:

h	β^+	β^-	error	ratio
0.100	1000	1	2.227782D - 04	---
0.050	1000	1	5.391984D - 05	4.13
0.025	1000	1	1.307318D - 05	4.12

Table 5.1

h	β^+	β^-	error	ratio
0.100	1	1000	2.392997D - 05	---
0.050	1	1000	6.703319D - 06	3.57
0.025	1	1000	1.766744D - 06	3.79

Table 5.2

h	β^+	β^-	error	ratio
0.100	5	1	2.629529D - 04	---
0.050	5	1	6.351060D - 05	4.14
0.025	5	1	1.550294D - 05	4.10

Table 5.3

h	β^+	β^-	error	ratio
0.100	1	5	5.461059D - 05	---
0.050	1	5	1.309861D - 05	4.17
0.025	1	5	3.263757D - 06	4.01

Table 5.4

The tables show that when h is reduced to a half of it, the error is reduced approximately to a quarter of it. That confirms the numerical solution has second order accuracy.

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